Butanoic anhydride

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.28

Global applicability domain: Inside

Local applicability domain index: 5.78e-01

Confidence level: 8.18e-01

Nearest Neighbors from the Training Set

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tert-Butyl acetate
Measured: 1.76
Predicted: 1.61

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4-Methyl-2-pentanone
Measured: 1.31
Predicted: 1.43

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2-Hexanone
Measured: 1.38
Predicted: 1.42

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3,5-Heptanedione
Measured: 1.12
Predicted: 9.07e-01